Hybrid Dynamic Modelling of Engine Emissions on Multi-Physics Simulation Platform

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Abstract. This paper introduces a hybrid dynamic modelling approach for the prediction of NOx emissions for a Diesel engine, based on a multi-physics simulation platform coupling a 1-D air path model (GT-Suite) with in-cylinder combustion model (CMCL Stochastic Reactor Model Engine Suite). The key motivation for this research was the requirement to establish a real time stochastic simulation capability for emissions predictions early in engine development, which required the replacement of the slow combustion chemistry solver (SRM) with an appropriate surrogate model. The novelty of the approach in this research is the introduction of a hybrid approach to metamodeling that combines dynamic experiments for the gas path model with a zonal optimal space-filling design of experiments (DoEs) for the combustion model. The dynamic experiments run on the virtual Diesel engine model (GT- Suite) was used to fit a dynamic model for the parameters required as input to the SRM. Optimal Latin Hypercubes (OLH) DoE run on the SRM model was used to fit a response surface model for the NOx emissions. This surrogate NOx model was then used to replace the computationally expensive SRM simulation, enabling real time simulations of transient drive cycles to be executed. The performance of the proposed approach was validated on a simulated NEDC drive cycle against experimental data collected for the engine case study, which proved the capability of methodology to capture the transient trends for the NOx emissions. The significance of this work is that it provided an efficient approach to the development of a global model with real time transient modelling capability based on the integration of dynamic and local DoE metamodeling experiments.

Keywords: Engine Modelling, Dynamic Modelling, Emission Modelling, LOLIMOT, Local Model Networks, SRM

1 Introduction

Computer aided virtual engineering methods are playing an increasingly significant role in the engine development during preliminary stages of product development. This is enabled by significant cost and time compression achieved by replacing traditional testing and validation on physical prototypes during initial stages with high fidelity simulation models. The application of CAE system models for internal combustion engine is exemplified by the virtual engine prototypes which combine air path models with combustion process model to enable complete engine simulation during early stages of development and replaces engine testing as the basis for mapping and calibration experiments.

This is an area of current research, as high-fidelity simulation models such as three-dimensional Computation Fluid Dynamics (3D-CFD) models are computationally expensive and require considerable time to converge. While data-driven models for emissions [1–4] are now common practice, these are not available during preliminary development phase due to their dependency on the engine testbed data. A significant advancement has been enabled by the introduction of Probability Density Function (PDF) based Stochastic Reactor Thermodynamic Models (SRM) [5–7], which can provide reasonably fast computation using the reduced chemistry mechanism, with a computation time of 2-3 minutes per cycle, while still preserving good prediction capabilities [8]. Although being relatively faster compared to the expensive 3D-CFD model, the SRM models still do not afford real time simulation capability. The industrial requirement, which demands real time simulation capability to evaluate driveability and emissions performance against legislative drive cycles, require methods which complement each other to strike a balance between high prediction quality and lower cost.

A preferable strategy would be to replace expensive simulation models with approximation models that are more efficient to run. These approximation models are referred to as metamodels (“model of a model”) [9] or surrogate models. The methodology for developing metamodels (metamodeling) is based on response surface modelling techniques [10] initially introduced to develop prediction models for expensive physical experimental responses [11]. Metamodeling is frequently and increasingly used in various fields as an alternative to expensive simulation models [12], with an increased diversity of models (polynomials, radial basis functions, kriging) [13] and physics based CAE analysis.

Korsunovs [14] has developed a Multi-Physics Engine Simulation (MPES) framework for a Diesel engine, that combines one-dimensional fluid dynamics model for air path model with Probability Density Function based Stochastic Reactor Thermodynamic model (SRM) for the combustion process. In order to develop real time emissions prediction capability, the approach in [14] was to replace the slow combustion chemistry solver (SRM) with an appropriate surrogate model, derived from DoEs on the virtual engine model that replicated the steady state experiments normally carried out during the engine development. However, many researchers [15–17] discussed that the practices of the steady-state process do not always transfer well to dynamic processes.

Furthermore, due to multiple engine operating modes (steady-state and transient) and challenges imposed by legislation such as transient emission regulations, steady state modelling process would be expensive to represent the transient behavior, as data need to be captured at an increased number of reference point for each of the multiple control parameters. Therefore, to incorporate the transient behavior into virtual engine prototypes and still being able to meet the industrial requirement (quality, cost, and time) during initial stages of engine development, a novel hybrid dynamic modelling approach for modelling engine emissions is introduced in this work.

The underlying principle of the proposed , Hybrid Dynamic Modelling framework in conjunction with the MPES platform, is to integrate dynamic modelling (using dynamic design of experiments and identification based models) with a global exploration-based design of experiments strategy to develop a global model for emissions. The proposed framework develops surrogate models for the two principal components of MPES, air path model and combustion process model. This is achieved by coupling two distinct metamodeling approaches; dynamic modelling techniques to develop a dynamic surrogate model for virtual engine air path, providing the input for a zonal design of experiments to develop metamodel for engine-out emissions (focusing on NOx) based on the combustion process simulation model. The effectiveness of the proposed framework is validated through an engine case study, as a proof of concept, focusing on a specific region of the engine operating domain.

One of the contributions of the research presented in this paper lies in the efficient development of metamodel capable of predicting transient drive cycle behavior during preliminary stages and enhancement of real time performance by incorporating dynamic modelling techniques. The latter arises from the fact that conventional methods for engine data collection are generally based on steady-state methods, which requires time to stabilize the engine before recording any data. Consequently, this takes a considerable amount of time. In this study, a MPES is used as virtual engine simulation platform where GT-Suite air path model (1D-model) provides air path states as response, which are then utilized as inputs to SRM combustion process model to estimate engine-out emissions (NOx emissions being the focus of this study). By implementing the proposed hybrid dynamic modelling framework, where 1D-model is replaced by surrogate model (dynamic air path model), the time taken to evaluate the air path states was dramatically reduced. A DoE of 170 points was implemented, both on the 1D-model and surrogate model (dynamic air path model), to generate inputs for SRM model and it was observed that 1D-model requires more than two hours to provide mean-value estimates for the air path states (model reaches steady state in 15-20 seconds). While on the other hand, surrogate model (dynamic air path model) was able to do the same in less than one minute. Also, the incorporation of dynamic metamodel would allow use of detailed models in Fast Response Model (FRM) applications without the need of reducing the model, i.e. simplify pipe, heat transfer in cylinder etc. Although the proposed methodology is presented in the context of emissions modelling, the fast simulation speed of the resulting models allows their implementation in context such as hardware-in-the-loop (HiL) systems to enable model based calibration of ECU [18]. Also, the resulting models can be utilized to perform analysis on different transient cycles or adapted for vehicle variants to suit the engineering requirements.

The structure of the paper includes a review of existing literature in section 2, followed by introduction of the proposed methodology in Section 3 along with the engine case study and evaluation criteria. Sections 4 and 5 present the implementation of proposed framework to develop metamodels of air path system and combustion process. The validation of the framework is detailed in section 6, and the paper concludes with the discussion of results and future work.

2 Review of Dynamic Modelling

There has been increasing interest in techniques for modelling dynamic behavior due to challenges imposed by legislation (such as transient emission regulations/ fuel economy reduction/ optimizing driveability for load changes) and multiple engine operating modes (steady-state and transient. This has led to a rise in efforts placed on investigation of dynamic calibration methodologies [1,19–21] and application of dynamic experiments and modelling techniques for the system modelling task [2,3,22–26]. The reason for these developments was underpinned by the possible advantages of these techniques such as faster data capture as no settling time is needed; improved model fidelity by capturing dynamic behavior; and inherent interpolation. The research in dynamic modelling can be categorized into two main categories:

- design of dynamic experiments,

- identification of dynamic models.

2.1 Design of Dynamic Experiments

For design of dynamic experiments, the popular choices are pseudo random binary signals (PRBS), amplitude modulated pseudo random binary signals (APRBS) and varying frequency sinusoidal signals (chirps). The PRBS sequence only alternates between the minimum and maximum value, this leads to poor coverage of input space [19], thus, makes the signal not suitable for the nonlinear system identification as no information regarding the system behavior is gathered other than at maximum and minimum points. This drawback is addressed by the APRBS type signals which vary in their amplitudes leading to better data coverage over a wide frequency range. However, the harsh nature of the step changes of these types of signals are not suitable to all systems and could be problematic for safe engine operation.

In this regard, the continuous nature (slow varying dynamic) of the chirp signals make them less problematic with regards to safe engine operation as they do not include step disturbances [2,27]. However, the disadvantage of the chirp signal is the scarce coverage of the center of the input space [26], thus, they require a long measurement time in order to cover the whole input space which increases with the number of relevant inputs. Application of these identification signals in literature is listed in **Table 1** and a generic illustration of these three type of excitation signal is depicted in **Fig. 1.**

Table 1. Overview of dynamic experiments applications in literature.

Excitation Signal	Modelling Approach	Application
Chirps	Volterra series	Engine Emissions [2]
Chirps	Volterra series/ MLP/ Hammerstein-wiener Model/ RBF/ NARX Model	Engine Emissions [27]
Chirps	Volterra Series	Exhaust Temperatures [25]
APRBS	Local neuro-fuzzy model	NOx Emission [28]
APRBS	Local neuro-fuzzy model	NOx Emissions [29][30]
Multi-sine/ Chirp/ Ramps	Gaussian Process Regression	Fuel Supply control system [31]

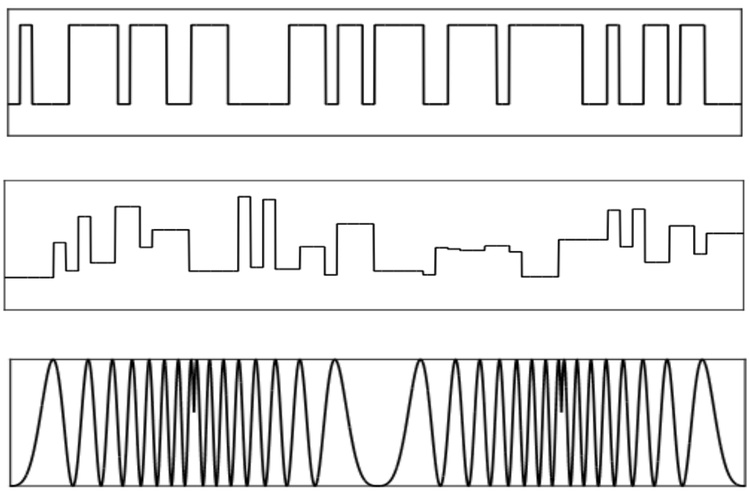


Fig. 1. Illustrations of common excitation signals: PRBS (top); APRBS (centre); Chirp (bottom).

There are range of non-linear dynamic modelling techniques which can be applied for modelling internal combustion engines. These modelling techniques define the mathematical relationship in between input and output without trying to adopt the physical system structure. These techniques have been widely implemented in the literature related to engine modelling such as Volterra series for prediction of emissions in [2,27], neural networks for modelling torque and lambda and fuel optimization in [32], modelling of Diesel engine with neural networks in [33], and NOx modelling using local linear neuro-fuzzy model in [34] and [30].

In existing work by the authors, a co-modelling strategy was presented which allows to select a signal and modelling technique combination suitable for the system modelling task [35]. For the co-modelling strategy, a combination of different excitation signal (PRBS/APRBS/chirps) with different identification techniques (Local linear neuro-fuzzy modelling/Neural Network) were studied for the same engine as in this research. The chosen model-signal combination was selected by comparing coefficient of determination (R^2), training & validation Root Mean Square Error (RMSE) and correlation between model prediction and system response. Based on these criteria, it was established that the APRBS with local neuro fuzzy modelling technique performed better than the other combinations for the system modelling task. Therefore, this combination is also selected in this work.

2.2 Local Linear Neuro-Fuzzy Modelling

The local linear neuro fuzzy (LLNF) modelling approach is based on the divide and conquer strategy. The most important factor for the success of such an approach is the division strategy for the original complex problem. Therefore, the properties of local linear neuro-fuzzy models crucially depend on the applied construction algorithm that implements a certain division strategy. The construction algorithm implemented in this research is Local Order Linear Model Tree (LOLIMOT) [36]: a multi-model approach which utilizes incremental partitioning strategy of axis orthogonal nature. The partitioning strategy and global structure of LOLIMOT is illustrated in **Fig. 2**. The model architecture has one hidden layer which consists of fuzzy neurons and one linear output layer. In this iterative modelling technique, for each iteration a new local linear model (LLM) is added [19]. These local models (LMs) are associated with the partition of the operating space, where they are valid, which is determined by the tree construction algorithm utilizing axis orthogonal splits [1].

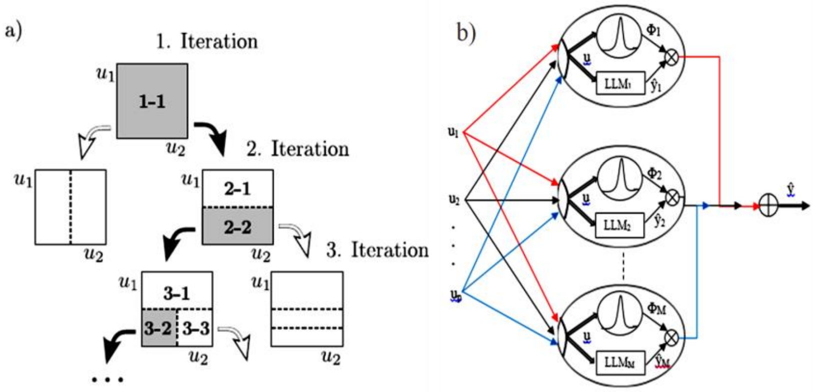


Fig. 2. a) Tree construction algorithm and its partitioning strategy and b) model structure of LOLIMOT illustrating the contribution of LLM towards the global model output.

The output of each LLM is given as:

$$\hat{y}_i = w_{i0} + w_{i1}u_1 + w_{i2}u_2 + \ldots\ldots + w_{ip}u_p \tag{1}$$

where w_{ij} denote the LLM parameters for neuron i [19] and $u = [u_1\ u_2\ \ldots u_p]$ is the input space vector.

The sum of the outputs of each LLM weighted by a validity function, Φ_i, leads to the global output ($\hat{y}$) of LLNF models and is given as:

$$\hat{y} = \sum \underbrace{\left(w_{i0} + w_{i1}u_1 + w_{i2}u_2 + \ldots\ldots + w_{ip}u_p\right)}_{\hat{y}_i} \Phi_i(\underline{u}) \tag{2}$$

The network interpolates between different LLMs with the validity functions (Φ_i) and generally validity functions are normalised Gaussian functions which depend on centre coordinates (c_{ij}) and standard deviations (σ_{ij}) [19], given as:

$$\Phi_i = \frac{\mu_i(\underline{u})}{\sum_{j=1}^{M} \mu_j(\underline{u})}$$

$$with\ \ \mu_i(\underline{u}) = \exp\left(-\frac{1}{2}\frac{(u_1-c_{i1})^2}{\sigma_{i1}^2}\right) \dots exp\left(-\frac{1}{2}\frac{\left(u_p-c_{ip}\right)^2}{\sigma_{ip}^2}\right) \quad (3)$$

The generic form of the local linear neuro fuzzy model described in (2), possess identical input space $u = \left[u_1\ u_2\ \dots u_p\right]^T$ for both rule consequents (local linear models) and premises (validity function). However, for local linear neuro fuzzy models, premises and consequents do not have to have identical variables and thus (2) can be extended to

$$\hat{y} = \sum_{i=1}^{M}\left(w_{i0} + w_{i1}x_1 + w_{i2}x_2 + \dots\dots + w_{i,nx}x_{nx}\right)\Phi_i\left(\underline{z}\right) \quad (4)$$

where local linear models depend on $\underline{x} = [x_1\ x_2\ \dots x_{nx}]^T$ and validity function depends on $\underline{z} = [z_1\ z_2\ \dots z_{nz}]^T$. This represents the static form of the local linear neuro fuzzy model, a dynamic local linear neuro fuzzy model, for p number of inputs and m order, can be obtained by setting rule consequent input vector ($\underline{x}$) and rule premises input vector $\left(\underline{z}\right)$ as:

$$\underline{\mathrm{x}} = \underline{\varphi}(\mathrm{k}), \quad \underline{\mathrm{z}} = \underline{\varphi}\mathrm{k} \quad (5)$$

$$with\ \ \underline{\varphi}(\mathrm{k}) = \begin{matrix}[\mathrm{u_1(k-1)} \dots \mathrm{u_1(k-m)} \dots \mathrm{u_p(k-1)} \dots \mathrm{u_p(k-m)} \\ \mathrm{y(k-m)} \dots \mathrm{y(k-m)}]\end{matrix}^{\mathrm{T}} \quad (6)$$

where $\underline{\varphi}(k)$ is the vector containing regressors. By incorporating (5) and (6), a dynamic local linear neuro fuzzy model for single input can be written as

$$\hat{\mathrm{y}}(\mathrm{k}) = \sum_{\mathrm{i=1}}^{\mathrm{M}}\{\mathrm{b_{i1}u(k-1)} + .. + \mathrm{b_{im}u(k-m)} - \mathrm{a_{i1}}\hat{\mathrm{y}}(\mathrm{k}-1) - \dots \mathrm{a_{im}}\hat{\mathrm{y}}(\mathrm{k-m}) + \zeta_{\mathrm{i}}\}\Phi_{\mathrm{i}}\left(\underline{\mathrm{z}}\right) \quad (7)$$

where b_{ij} and a_{ij} represent the numerator and denominator coefficients, ζ_i is the offset of the i^{th} local linear model and M denotes the number of local linear models. The ability to assign different input vector for validity function and local linear model is one of the strength of local linear neuro fuzzy modelling [19]. However, if no prior knowledge is available regarding the system, same input vector is chosen for both consequents and premises.

3 Methodology

The principle of the proposed hybrid dynamic modelling approach based on the multi-physics engine simulation framework (MPES) is presented in **Fig. 3**. The MPES virtual engine simulation framework, highlighted in the top section of **Fig. 3**, combines air path simulation model (GT-Suite 1D-model) with a combustion chemistry solver (SRM) which describes the combustion process. Engine mapping and calibration experiments based on the MPES platform could be in principle similar to the model based calibration (MBC) strategy of running steady-state experiments on a physical engine.

It is important to note that the GT-Suite model accounts only for the air path variables, not involving any chemical calculations. In order to account for the combustion phenomena within the cylinder, experimental heat release rate (HRR) profiles are used to predict the in-cylinder pressure, but the model cannot predict engine-out emissions. The SRM combustion models have proven capability [5] for in-cylinder emissions predictions based on boundary conditions, which could be either from engine experiments or virtual engine air path simulations – in this case provided by the GT-Suite model. While the GT-Suite air path model runs in real-time with good accuracy, depending on the complexity of the model, the SRM combustion solver requires significant computation expense, and therefore an overall real time simulation capability is not immediately possible.

The proposed hybrid dynamic modelling framework aims to overcome this challenge by replacing the GT-air path model with a surrogate model, which would provide the air path states as input to the SRM combustion model. Thereafter, SRM model being replaced by a surrogate emissions model developed by fitting statistical model on SRM predictions. A research challenge is to design an efficient experimentation strategy to enable the development of a global metamodel at a cost comparable with the steady state experiments performed to develop the SRM surrogate model. To this end, a hybrid meta-modelling strategy is proposed, which couples two fundamentally different types of metamodeling strategies for the 2 structural parts of the MPES framework:

- A dynamic modelling / identification technique is deployed to develop a surrogate for the GT-Suite dynamic airpath simulation model of the Diesel engine (labelled as block 1 in **Fig. 3**);
- A global exploration DoE experiment, based on space-filling Optimal Latin Hypercube (OLH) DoEs, to develop a surrogate model for emissions – focusing on NOx engine-out emissions, based on the SRM model (labelled as block 2 in **Fig. 3**).

The integrated combination of the dynamic experimental modelling deployed to the real-time GT airpath model with the global OLH DoE experiment deployed on the SRM individual cycle emissions solver justifies the hybrid nature of the proposed approach. The surrogate model for the dynamic GT airpath model is needed to provide a fast mean-value estimate for the inputs required for the SRM model. The reason being in order to develop surrogate NOx emission model (based on SRM model NOx predictions), at cost comparable to steady-state modelling, would require capability to provide mean-value estimates of air path states faster than real time. By deploying the dynamic model for surrogate modeling of GT-air path model would deliver a considerable time saving, as otherwise, the GT model would have to be run for a considerable amount of time (15-20 seconds to reach stable steady state operation) to deliver a robust input for the global SRM experiments.

MPES – Multi-Physics Engine Simulation: Hybrid Dynamic Modelling Approach

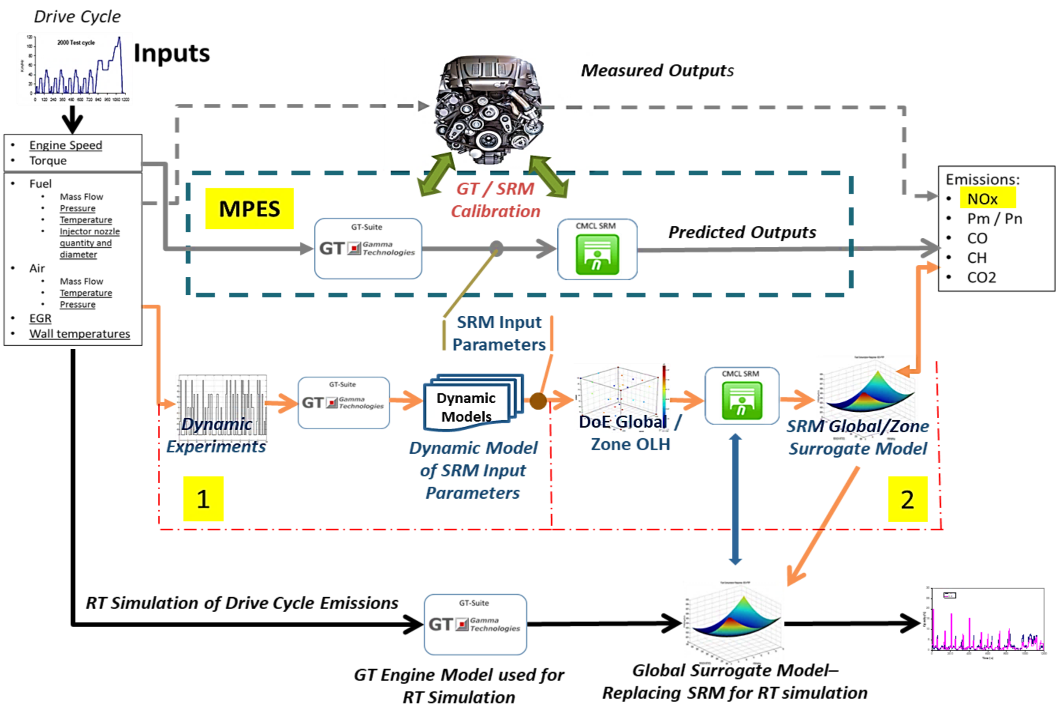


Fig. 3. Hybrid dynamic modelling approach based on MPES platform.

3.1 Engine Case Study

The engine case study for this research was a 4-cylinder 2.0-liter turbocharged Diesel engine with common rail injection technology, single variable geometry turbocharger, high and low pressure exhaust gas recirculation (EGR) systems, and water charge air cooler (CAC) set up as in test bed environment and controlled to a fixed value. The basic information regarding this engine is tabulated in **Table 2**. The experimentally validated GT-Suite engine model of a 2.0 L Euro 6c Diesel engine was available. The model was initially developed as a One-dimensional (1D) fluid dynamics model representing the air path of the Diesel engine and then converted into a fast running model (FRM) capable of running in real-time to act as a virtual engine for collecting data to train dynamic models. The probability density function (PDF) based stochastic rector model (SRM), developed by Korsunovs et. al. [5], was used to represent the combustion process model and is used to predict the emissions. In addition to this, New European Drive Cycle (NEDC) data measured on a transient engine dynamometer test facility was also available.

Table 2. Diesel Engine Basic Information

Parameter	**Value**
Bore	83 mm
Stroke	92.35 mm
Connecting Rod Length	140 mm
Compression Ratio	15.5
Emissions Standard	Euro 6c
Peak Power	130 kW @ 4000 RPM
Peak Torque	430 Nm @ 1750 – 2500 RPM
Combustion Modes	Standard-calibration combustion for experiments

3.2 Simulation Case Study

The task of developing the hybrid dynamic modelling framework was approached by partitioning of the operational domain of the available drive cycle data into smaller sections, zones, based on engine speed, as illustrated in **Fig. 4**. To allow smooth interpolation and gradual transition in between the global models identified at each zone, an overlap between the zones (soft partitioning) was introduced [37,38]. The rationale for this is that by decomposing modelling problem into zones, compliance to constraints for dynamic experiments can be taken into account more easily [24] and global models at zones could have better accuracy relative to global models generated on a wide range, as experiments can be planned to suit the needs of a particular zone [37].

A subset of the operating range for the selected zone (zone 3) that lies between engine speeds of 1500-1750 rpm and torque of 20-160.6 Nm was selected as focus for the study, with the aim to prove the validity of the methodology concept. This was facilitated by the availability of an accurate injector model [14] for this zone in the form of injection profiles capturing the injection characteristics. The suitability of this zone for the study can also be argued in relation to the observation of a good distribution of both low and high loads across the operating range of this zone. The load band selected is representative, as it covers a wide range where engine operates in NEDC drive cycle. While this does not directly relate to the engine speed, it is still an acceptable range as the engine does commonly operate in the selected speed band. Given the main purpose was to provide a proof of concept validation for the proposed methodology, the selected zone is suitable for the objective of NOx emission modelling given load affects NOx more significantly than speed.

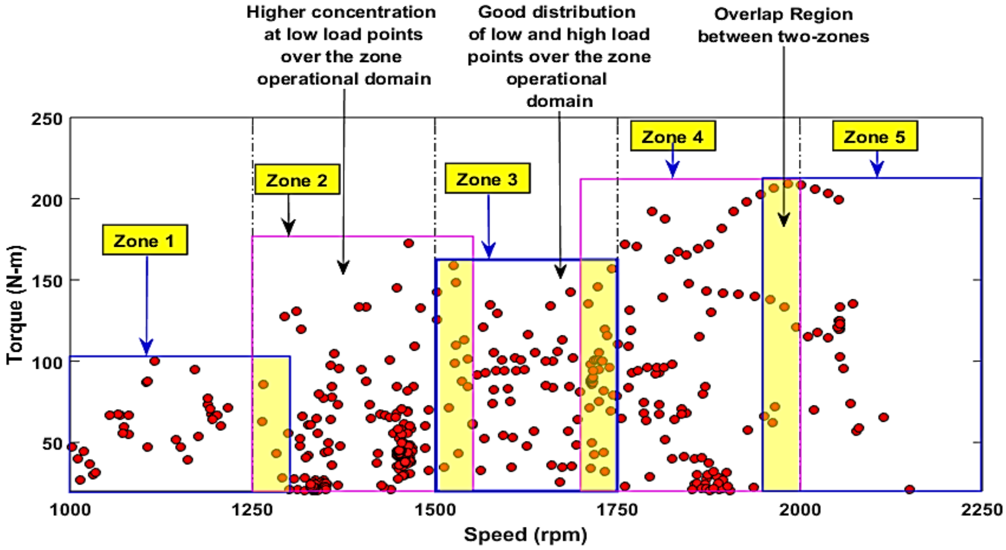


Fig. 4. Operational domain partition of the drive cycle based on engine speed.

3.3 Model Evaluation

The quality of surrogate air path model was evaluated using fit statistics detailed by Root Mean Square Error (RMSE), and normalized RMSE (nRMSE) according to

$$\mathrm{RMSE} = \sqrt{\frac{1}{n} \cdot \sum_{i=1}^{n} (y_i - \hat{y}_i)^2} \tag{8}$$

$$\mathrm{nRMSE} = \frac{\mathrm{RMSE}}{\max(y_i) - \min(y_i)} \times 100 \tag{9}$$

For surrogate combustion modelling following fit statics, Prediction Error Sum of Squares-RMSE (PRESS-RMSE) and relative error, were employed.

$$\text{PRESS-RMSE} = \sqrt{\frac{1}{n} \cdot \sum_{i=1}^{n} (y_i - \hat{y}_i)^2} \tag{10}$$

$$\text{Relative Error (\%)} = \frac{RMSE}{\bar{y}} \times 100 \tag{11}$$

These statistical criterions provide information about quality of model if applied to prediction of training data whereas they give measure of predictive performance if applied to validation data (new set of data not used in training). If there is a significant difference in between the model prediction for training and validation data, this is a sign that model is over-fitted.

4 Surrogate Dynamic Air Path Model

4.1 Model Inputs and Outputs

The methodology for development of surrogate airpath model presented here closely follows the work presented by the authors in [35]. The dynamic metamodel for the 1D airpath model was developed to provide a fast mean value estimate for the combustion model inputs. The desired engine speed and load were selected as control variables for the identification of the dynamic air path as these two quantities are required to simulate the GT-suite engine model. In addition to these two, Mass Air Flow was also selected as it controls the EGR valve position in a closed loop, which regulates the amount of exhaust gas entering the engine cylinder.

The excitation method and the range for input variables is defined in the **Table 3**. The excitation range, for the desired engine speed and load, was defined by the operational limit of the simulation case study zone. For MAF, the limit was set to be ± 10% of MAF set position (from calibration maps in ECU), to account for the variation in between transient and steady-state modes of operation. In addition to excitation range, frequency range was defined based on the frequency analysis of the drive cycle data and is tabulated in **Table 3**.

In Korsunovs *et. al.* [5], it was established that three air path states, inlet pressure (*P_inl*) / inlet temperature (*T_inl*) or intake manifold temperature / overall EGR mass fraction (*EGR_mf*), have a significant effect on the NOx prediction while the other external parameters did not have any effect or not significant enough. Thus, these three quantities were selected as response to be modelled.

Table 3. Input parameters for surrogate dynamic air path model.

Inputs	Excitation Method	Excitation Range	Frequency Range
Engine Speed	Direct control through Simulink harness for 1D airpath model	1500-1750 rpm	0.003-0.1Hz
Engine Load	Control through the transformation of torque setpoint to fuel injection quantity via pre-defined maps	20-160.6 Nm	0.01-0.1 Hz
Mass Air Flow	Control through mass air flow set point in ECU. This is because EGR is in closed loop control depending on the MAF demand.	±10%	0.001-0.06Hz

The APRBS type excitation signals generated for training based on the configuration listed in **Table 3** are illustrated in **Fig. 5**. The signals are designed individually for each input. However, this will result in operating points that are not achievable in practice because of limitations either in terms of mechanical integrity of the engine or because of operation in unstable conditions [2]. To account for this, the engine torque signal has been continuously scaled as a function of engine speed. In **Fig. 5**, the solid line stands for original torque and dashed line is signal after scaling.

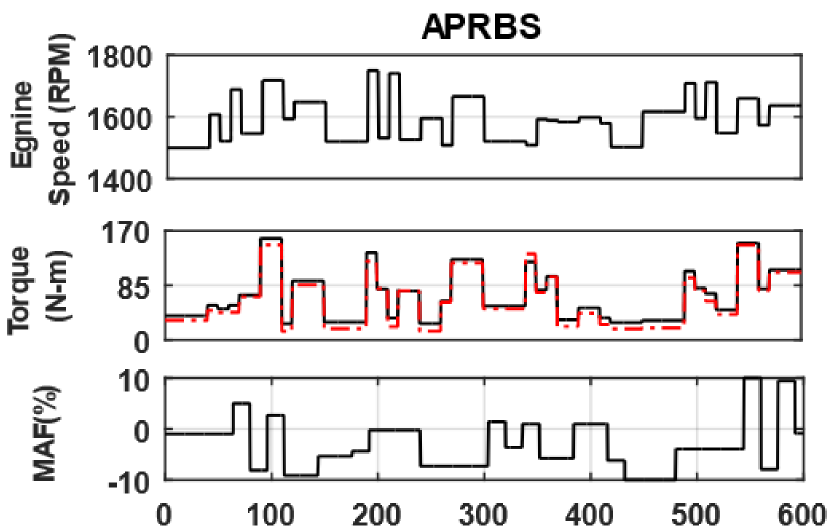


Fig. 5. APRBS training input signals (dash: scaled signal & solid: original signal).

4.2 Development of Diesel Engine Dynamic Air Path Model

The dynamic air path metamodel is developed by data obtained from dynamic tests (illustrated in **Fig. 6**) in virtual diesel engine air path (GT-Suite) model. This stage is illustrated in **Fig. 3**, where excitations signals are fed to virtual Diesel engine air path of MPES platform, and the system responses of interest are captured. The inputs signal along with the outputs are used for training the dynamic models.

In this paper, a dynamic local linear neuro-fuzzy model (Lolimot) was chosen as the dynamic model format. Since models are used for simulating the air path output rather than predicting the output k-step ahead, parallel model structure is selected which simulates the current output by input and previously simulated output. The local model network is constructed in conventional manner with one hidden layer and a single output layer. The number of local linear models is determined by the Lolimot construction algorithm (training procedure illustrated in **Fig. 7**) based on the improvement in modelling accuracy and number of parameters.

The input and output delays should be optimized to give the best trade off model between model accuracy and complexity. As multiple dimension optimization can be time consuming, in this study they are selected by trial-and-error tests on few settings.

Dynamic air path was modelled as nonlinear Multiple Input Single Output (MISO) system and models of the selected response quantities, *EGR_mf / P_inl / T_inl*, were developed and relational form is given as follow:

$$\hat{y}_{EGR}(\mathrm{k}) = f(u_1(k-1), u_1(k-2), u_2(k-1), u_2(k-2), u_2(k-3), u_3(k-1), u_3(k-2), u_3(k-3), y(k-1), y(k-2)) \quad (12)$$

$$\hat{y}_{pressure}(\mathrm{k}) = f(u_1(k-1),\ u_2(k-1), u_3(k-1), y(k-1), y(k-2)) \quad (13)$$

$$\hat{y}_{Temp}(\mathrm{k}) = f(u_1(k),\ u_2(k-1), u_3(k-1), y(k-1), y(k-2), y(k-3)) \quad (14)$$

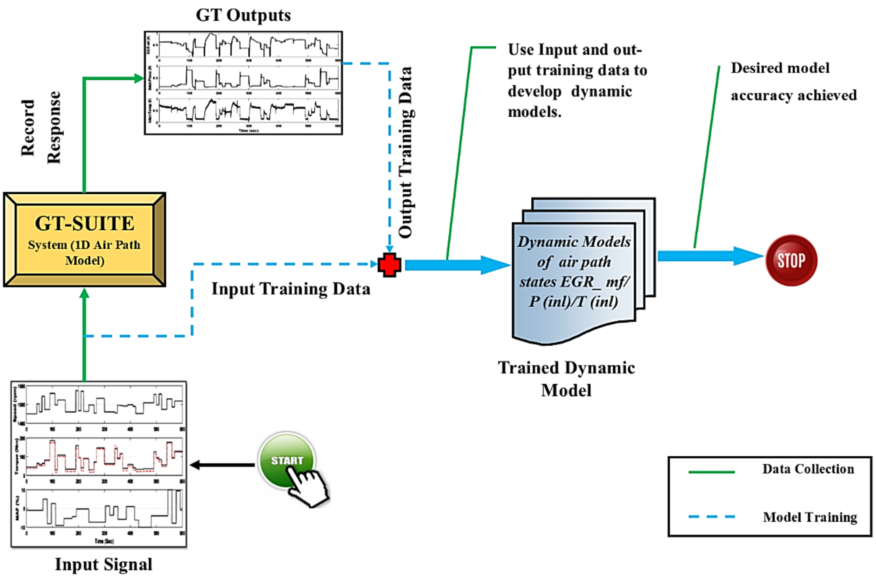


Fig. 6. Training process during the development of the dynamic air path model.

Step 1: Define Model Inputs and Outputs

Step 2: Start with the Initial Model

Construct the validity function, if no initial input space partitioning available set number of Local Linear models (LLM), M = 1 with validity function $\phi_1(u) = 1$. Estimate a global linear model $y = w_0 + w_1 x_1 + \cdots + w_n x_n$,.

Step 3: Find Worst LLM

For ***i*** = 1,…,M % LLM

a) Estimate Local Loss Function

$$I_i = \sum_{j=1}^{N} e^2(j)\phi_i(u(j))$$

b) Find the worst performing local model, i.e. $\max(I_i)$, and denote $'k'$ as the index of this worst LLM.

Step 4: Further refine worst LLM $'\boldsymbol{k}'$

a) Cut the hyper-rectangle into two halves, division in all dimension are tried (dim = 1,…,p).
b) Estimate local linear models for each half.
c) Calculate the approximation error (output error) for the model with this cut.
d) Determine which division, in p alternatives dimensions, has led to the smallest approximation error and select that division.

Step 5: Implement Best Division

Perform the division selected in step 3. Place a weighting function within each centre of both hyper-rectangles. Set standard deviations of both weighting functions proportional to the extension of the hyper-rectangle in each dimension. Apply the corresponding estimated local linear models (from 3b). The number of LLM is incremented $\boldsymbol{M} \rightarrow \boldsymbol{M} + \mathbf{1}$

Step 6: Test for Convergence

Convergence: If the termination criteria are met then stop, else go to step 2. Repeat until termination criteria are met.

Fig. 7. Identification of dynamic air path model using LLLNF modelling technique.

4.3 Results

The model predictions for the dynamic air path model for both training and validation are illustrated in **Fig. 8** and **Fig. 9** respectively. The correlation between all response quantities from virtual engine and Lolimot show a good match, for both training and validation, and follow the trends in the data.

In addition to this the quality of the model is quantified by the statistics summarized in the **Table 4**. The performance of the three response models is satisfactory for both training and validation datasets. The fit statistics observed for the temperature model is relatively higher when compared to the other two response models but is within the reasonable limits.

For the intake manifold temperature model results, the model accurately predicts the associated trends but has some limitations in capturing the rapid transients. This limitation with capturing transients could have an effect on NOx prediction, as increase in inlet temperature leads to higher combustion temperature, resulting in higher NOx. However, as the temperature increases, the density of air decreases, which results in lower amount of air mass trapped in the cylinder, and hence less cylinder pressure at the beginning of the combustion process. This counters, to a certain degree, the effect the increasing inlet temperature has on NOx. From the sensitivity analysis carried out by authors in [5], it was observed that one kelvin of change in temperature would lead to approximately 1.1 ppm change in NOx. The error in the inlet temperature model presented here, both for training and validation, is less than 3 Kelvin. This would imply approximately 3 ppm error in NOx, assuming the trend observed in the sensitivity analysis is more or less linear, which was within acceptable range for this study. This justifies the number of delay terms selected for modelling, (12) - (14), as they allow to accurately capture the dynamics associated with the response variables.

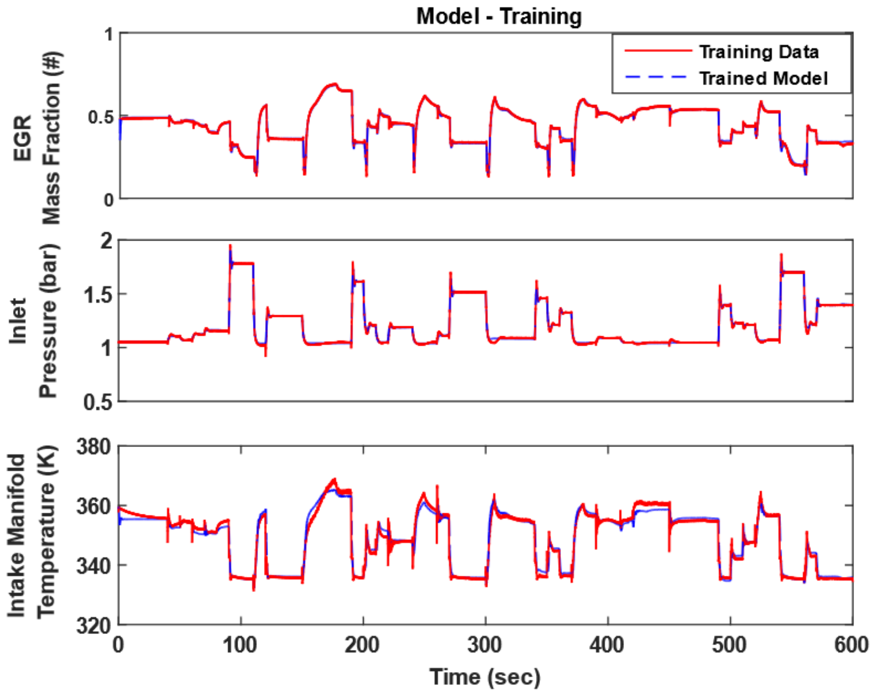


Fig. 8. Surrogate air path LOLIMOT model training performance.

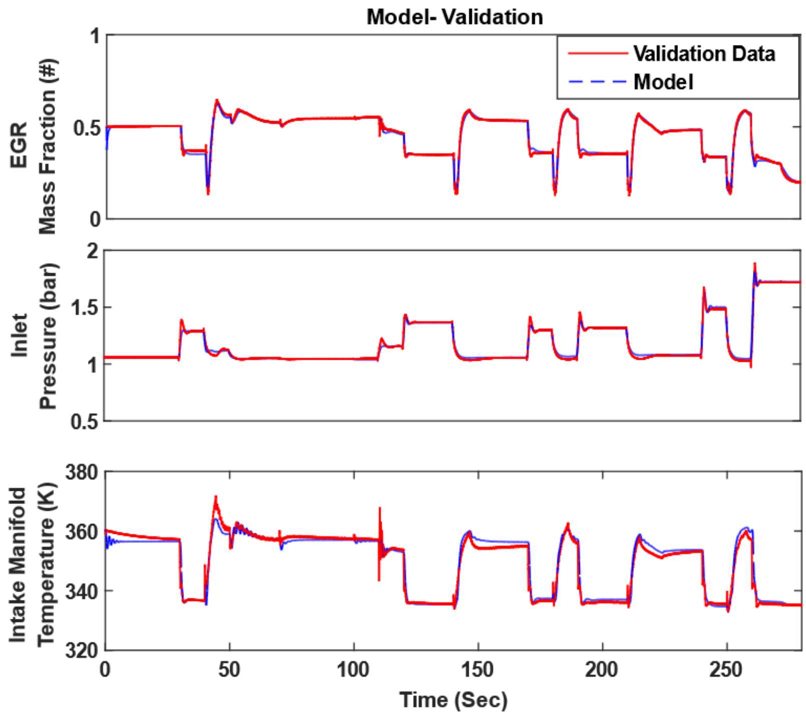


Fig. 9. Surrogate air path LOLIMOT model validation performance.

Table 4. Fit statistics for training and validation of the air path surrogate dynamic model.

Response Model	Units	Number of LLM	Training-RMSE	nRMSE	Validation-RMSE	nRMSE

EGR Mass Fraction	#	21	0.009	1.73 %	0.014	2.5 %
Inlet Pressure	Bar	12	0.011	1.1 %	0.017	2.2 %
Inlet Temperature	Kelvin (K)	14	1.882	5.0 %	2.124	6.8 %

5 SRM Combustion Process Model

The combustion process was modelled in the CMCL SRM environment and the chemistry mechanism for the model was chosen to be “Reduced Diesel with NOx”, which is CMCL internally developed mechanism. The CMCL SRM combustion solver sub-models and settings [14] are summarized in **Table 5**.

Details regarding the methodology for the SRM model calibration are discussed in detail in the previous work by the authors [5]. The calibration goal was to derive settings for the SRM parameters, such that a good correlation can be obtained with the engine testbed measurements and SRM model outputs. To proceed with the calibration task a detailed sensitivity analysis of the SRM model outputs, engine emissions (NOx) prediction and in-cylinder condition, in relation to SRM parameters was carried out in [5].

Table 5. CMCL SRM Sub-Models Settings

Sub-Model	Settings
Initial Mixture at the Inlet	• Oxidiser Composition (air surrogate): 76.7% nitrogen (N2), 23.3% oxygen (O2), • EGR composition auto-generated for the initial cycle, then updated from cycle to cycle.
Fuel and Injection	• PDF injection model (Fuel evaporation is described by the PDF) • No wall impingement • Elkotb SMD correlation • Imposed Injection Rate Profile • Surrogate Diesel fuel: 80% n-Heptane (C7H16), 20% iso-octane (C8H18)
Heat Transfer	• Woschni Heat Transfer Model • In-cylinder wall temperatures estimated from GT-Power
Turbulence	• Empirical k-epsilon Mixing Model

5.1 Surrogate NOx Model

The SRM combustion model developed and validated by the authors in [5] provides engine-out emissions as a response. While SRM combustion model provides results for all the engine out emissions, such as CO, HC, soot, NOx etc., this work focuses only on modelling of NOx. This is because the current SRM model is single zone thermodynamic model and present limitations in the prediction of other pollutants [14]. The combustion model used in this study, although relatively faster compared to the expensive 3D-CFD model, does not have real time simulation capability.

To overcome the limitation of SRM combustion model, to instantaneously predict NOx emission based on the air path conditions provided by the surrogate dynamic air path model, it is replaced by a surrogate NOx model. The said surrogate NOx model is a statistical model fitted to the NOx emissions response predicted by SRM during combustion. The modelling process involved in the development of a NOx surrogate model, the second stage of the proposed hybrid dynamic modelling approach is illustrated in **Fig. 10**, and can be summarized in the following few steps:

- Design of Experiment
- Data Collection
- Fitting Surrogate Model

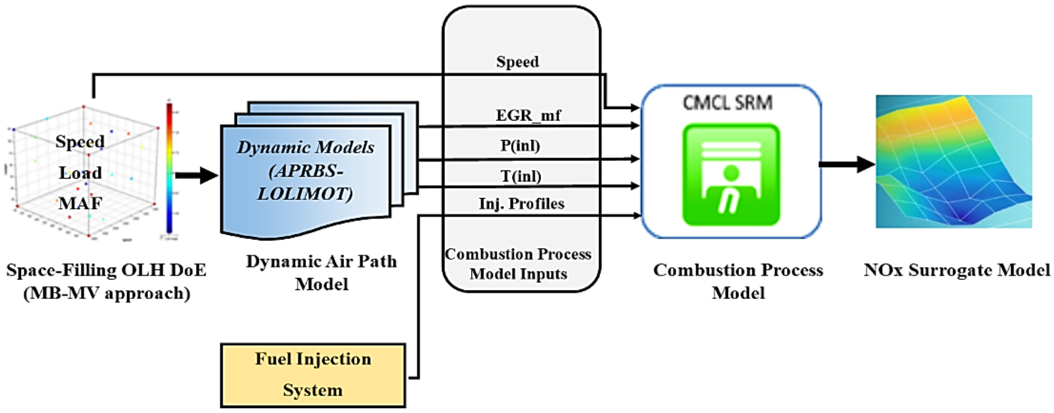


Fig. 10. Process of developing surrogate NOx model.

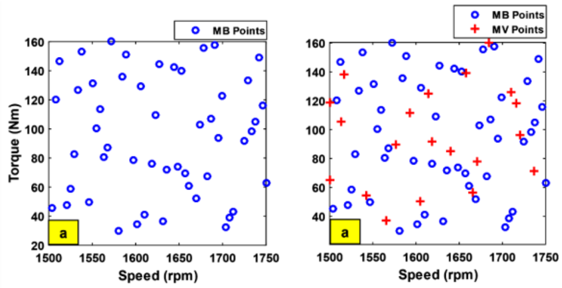
5.2 Design of Experiment

The model inputs considered for the development of the surrogate combustion model can be classified into three types depending on their point of origin:

- Operation Point Inputs: these inputs are directed from the engine operational domain. These inputs include engine speed and engine load (Torque): they represent the engine demand through the driving cycle.
- Intake Mixture Dynamics: these inputs are directed from the air path model and in this study from the dynamic air path model. In other words, the outputs of the dynamic air path model: *EGR_mf*; *P_inl*; *T_inl*.
- Intake Fuel Dynamics: the usage of common rail systems enables the variation of rail pressure and a splitting of the injection in the pilot, main and post injections. However, the settling of rail pressure has dynamics associated with it, but it is relatively fast [1], and is disregarded in this study. To account for the injection characteristics of the system, injection profiles were provided by the sponsor company, and these profiles were utilized for the combustion process model.

The design of experiments (DoE) approach used in this work is an exploration based sequential DoE strategy based on optimal space filling OLH design proposed by Kianifar et al in [39] and implemented into custom MATLAB toolbox [40]. The OLH based sequential DoE is a Model Building - Model Validation (MB-MV) DoE strategy, where a response model is fitted to the MB OLH DoE, and the quality of the model is evaluated, using internal and external information criteria, against the MV OLH DoE. By deploying this framework, the cost associated with the development of surrogate model could be minimized due to its property of terminating introduction of additional test points once the target accuracy is achieved. Thus, fitting the response surface model with the least possible number of test points.

The designed experiments, for an example **Fig. 11**, were plugged into the dynamic air path model (surrogate model) to generate intake mixture dynamics input (dynamic air path outputs) for combustion. In the process of surrogate NOx modelling, the MB-MV DoE strategy was applied in six iterations and design space for the first and sixth iteration is depicted in **Fig. 11**.



MB-MV sequence: a) MB, OLH of 50 points, b) plus points show the position of validation points (MV1), OLH of 20 points, among MB points

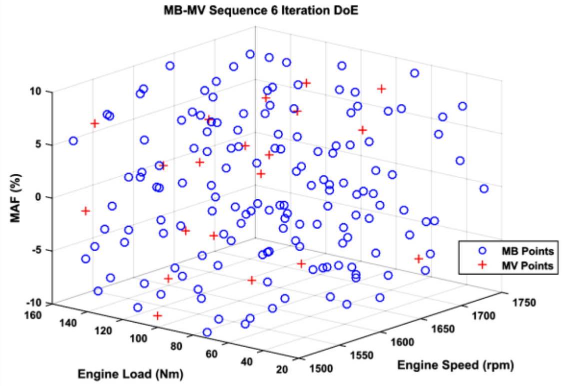


Fig. 11. Illustration of Design of Experiment: design space for the first and sixth iteration.

The DoE design quality was evaluated and it was observed (see **Fig. 12**) that the space filling property for the DoE was maintained after 6 iterations, where none of the generated test points (for both MB and MV) is too close to each other. Also, the correlation coefficient (r) for all the design parameters was within the range of $-0.04 \leq r \leq 0.04$, thus correlation is negligible. Therefore, the final design is quasi-orthogonal.

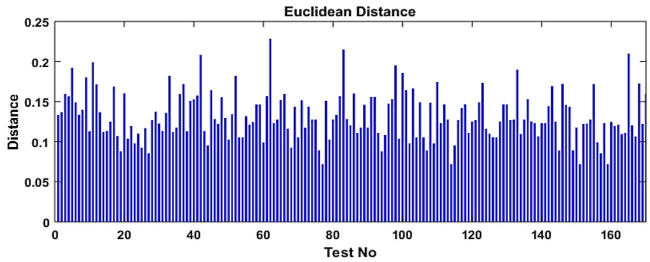


Fig. 12. Euclidean distance for all MB-MV test points (170 points).

5.3 Data Collection

The planned DoEs were plugged into the dynamic air path model and the SRM inputs captured by the surrogate model are illustrated in **Fig. 13**, along with the response from the GT-Suite Diesel engine model. It can be observed that the surrogate model predicts the trends in air path dynamics quite accurately.

The R-squared value illustrated in **Fig. 13**, indicates that the dynamic model of air path states input account for more than 95% of variance associated with the response of the system. The fitted line plot above illustrates that the model (dynamic model trained on dynamic signals) accurately (>96% fit for all three air path states input) describes the response for steady state points. In addition to the R-squared value, the statistical analysis of the prediction using validation RMSE (9) and relative error (12) is listed in **Table 6**. From the table, it can be observed that the dynamic models predict accurately for *EGR_mf* (<0.01 RMSE/1% *EGR_mf* or ~2% relative error), Inlet pressure (<1% relative error) and temperature (<1% relative error). This analysis illustrates that accuracy of the dynamic models developed earlier is not compromised for the different type of design of experiment approach, i.e. global OLH DoE (steady-state tests).

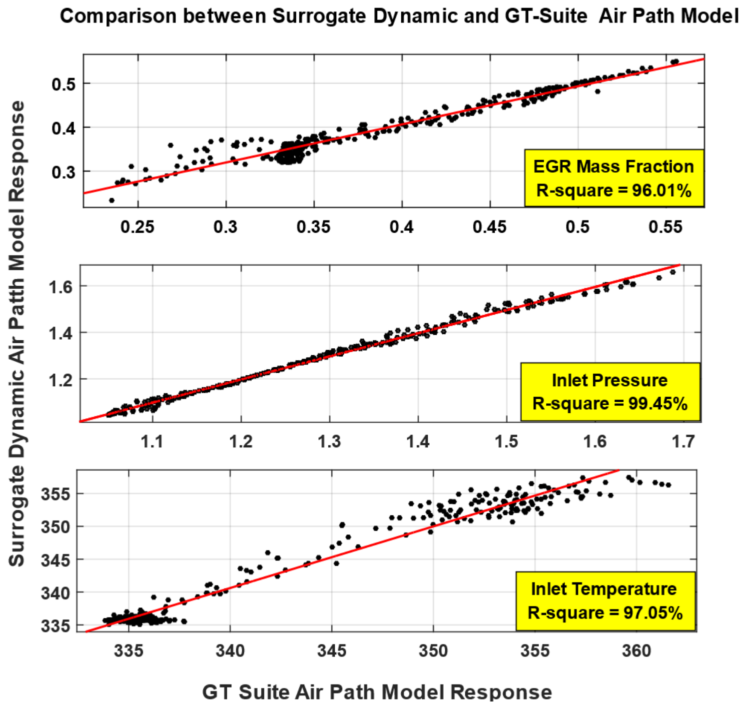


Fig. 13. Prediction of planned DoE by GT-Suite engine model and dynamic air path model.

Additionally incorporation of dynamic models also enhances the real time performance of the simulation model by reducing simulation time required (refer **Table 7**) to estimate the mean-value response of the inputs for the combustion process model. This reflects on the benefit of the hybrid dynamic modelling framework which incorporates a dynamic model for system modelling task, allowing quick modelling and fast data capture.

Table 6. Evaluation of performance of surrogate air path model on the DoE for SRM input parameters.

Model	Val_RMSE	% Relative Error
EGR	0.0084	2.1
Inlet Pressure	0.0026	0.20
Inlet Temperature	0.4146	0.12

Table 7. Simulation time to run steady state DoE.

Model	Simulation Time (sec)
GT-Suite Diesel Engine Model	8490
Surrogate Air Path Model (LOLIMOT-APRBS)	40

5.4 Development of Surrogate NOx Model

The procedure of the development of surrogate combustion model for predicting NOx emission is illustrated in **Fig. 14**. The figure depicts the procedure followed and presents the division of the process into stages. In this section of the paper the modelling stage is discussed, and its implementation is presented.

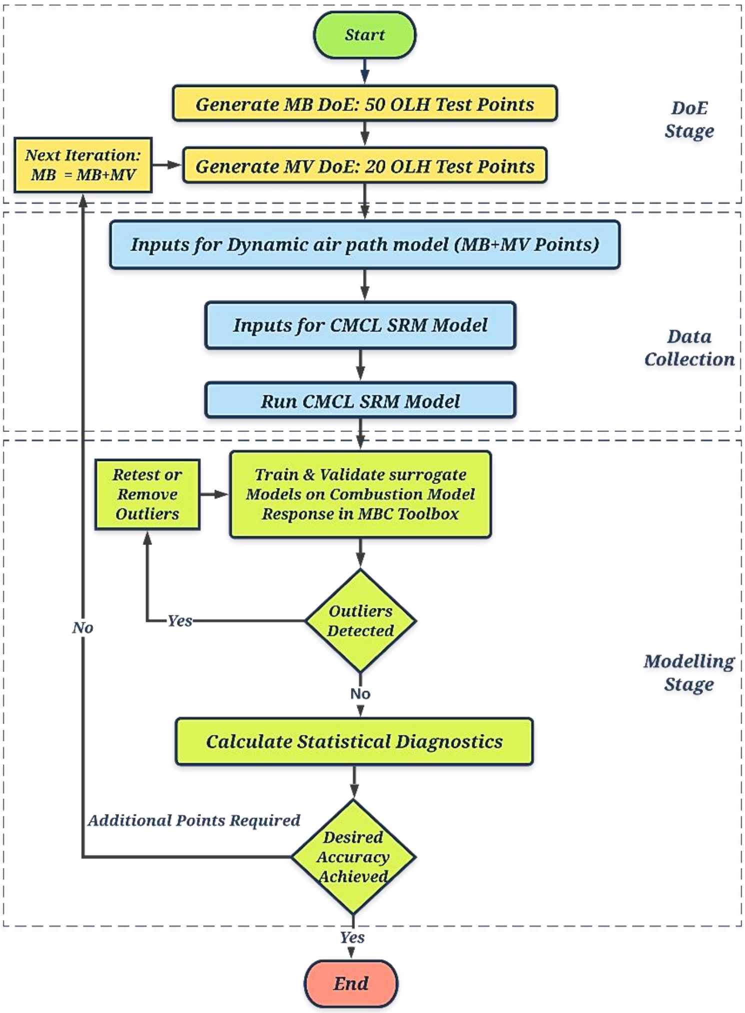


Fig. 14. The offline DoE and modelling strategy proposed for the metamodeling of combustion model.

In modelling stage of development process, response surface models are fitted to the NOx emission using MATLAB MBC toolbox. For every new iteration of DoE test plan, i.e. from MV1 to MV6, a new response model was fitted to the update system response. MATLAB MBC toolbox offers a range of statistical models for response surface modelling. Several combinations of response models, Polynomials, RBF with different kernels, Gaussian Process Models with different kernels, were fitted to the NOx emissions response.

The candidate models with various kernel functions were fitted to the first iteration of model building DoE with 50 test points. The comparison of prediction capability (PRESS RMSE) and the number of parameters required by each model are illustrated in **Fig. 15** and **Fig. 16** respectively.

From the **Fig. 15** and **Fig. 16**, it can be observed that Gaussian Process Model (GPM) with different basis function and kernels provides both good prediction capability and have a reasonable number of effective parameters. Amongst the GPM models, GPM with squared exponential basis function slightly performs better than the rest, therefore, is selected for further improvement with additional iterations of MB-MV DoE sequence.

The evaluation of the NOx surrogate model with a subsequent iteration of MB-MV sequential DoE (from MV1 to MV6) is illustrated in **Fig. 17**. The model was evaluated as per the information criteria, PRESS RMSE and Validation RMSE. It can be observed that the PRESS RMSE and Validation RMSE are decreasing, this indicates that the quality of the response model is improving with every new iteration of the sequential process.

The reason for this improvement comes from the fact that there are more infill or test points available for the response models to accurately capture the trends in the modelling data. The similar trend was observed in terms of relative error associated with the developed surrogate model and is depicted in **Fig. 18**. The relative error expressed here is the ratio of validation RMSE to mean response and is expressed as a percentage.

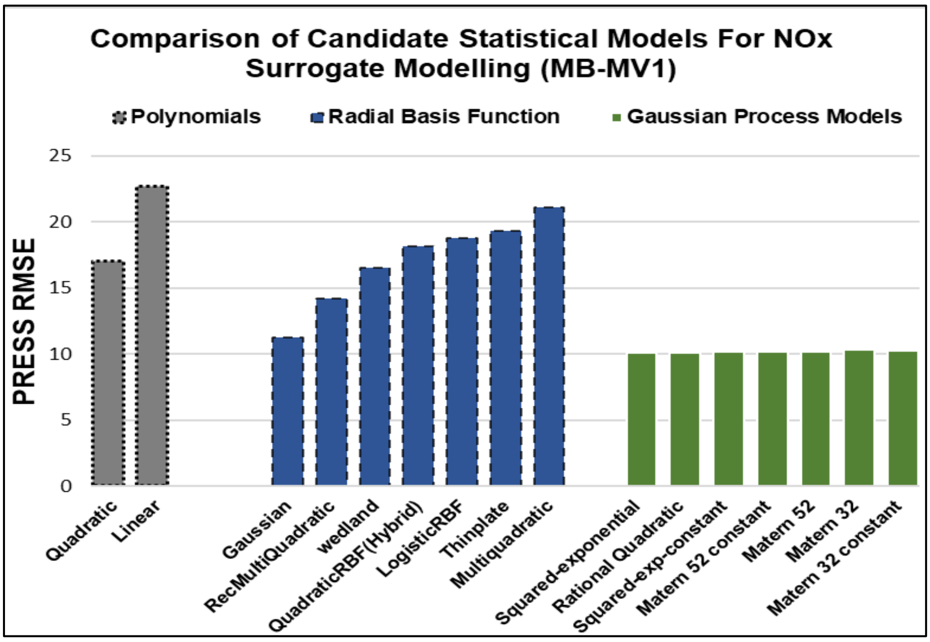


Fig. 15. Comparison of fitted response surface candidate models based on their prediction capability (PRESS RMSE) at MV1 iteration.

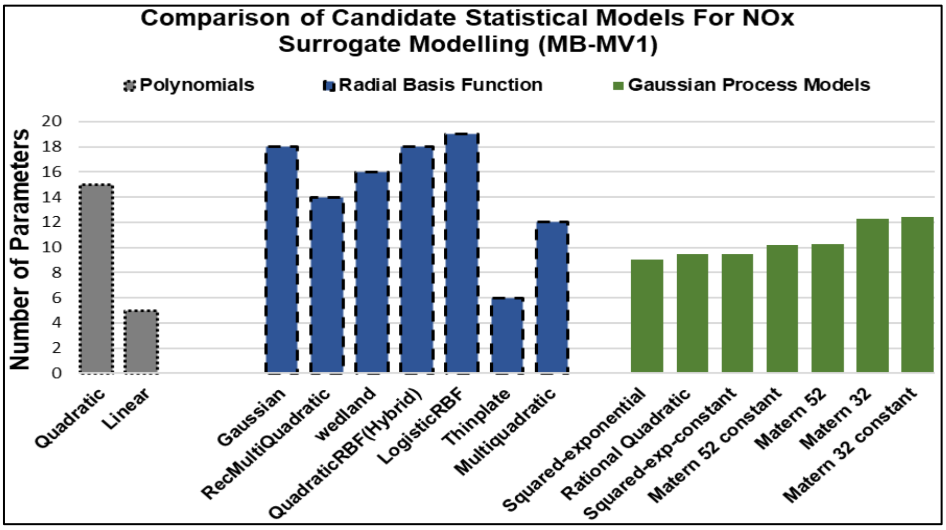


Fig. 16. Comparison of fitted response surface models based on the number of parameters required for modelling at MV1 iteration.

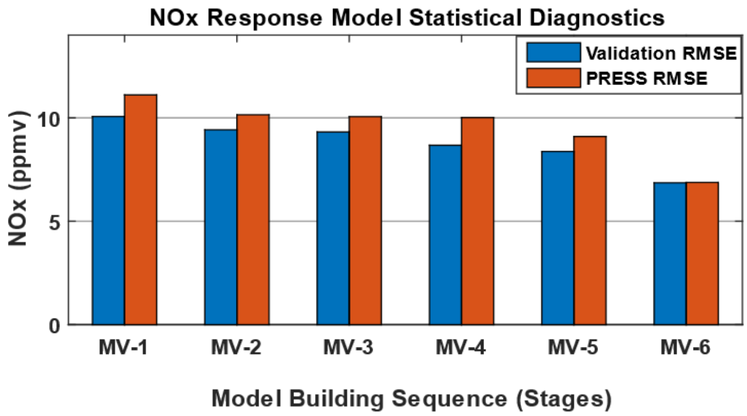


Fig. 17. PRESS RMSE and Validation RMSE for GPM NOx surrogate model during six stages/iteration of MB-MV.

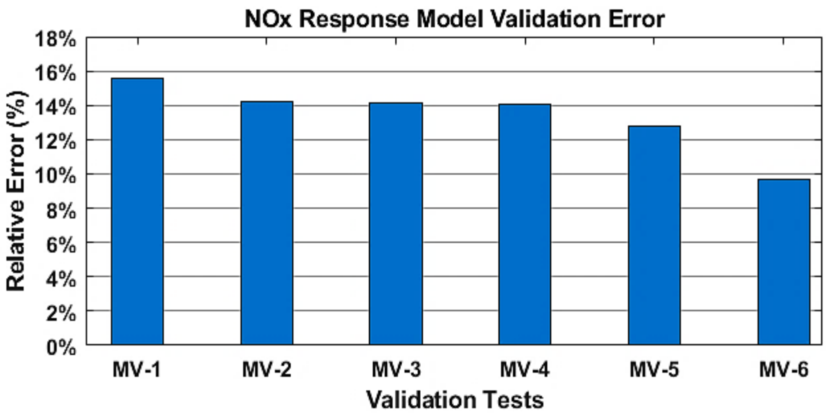


Fig. 18. NOx prediction relative error for all six stages of MB-MV sequential process.

The acceptable engineering target for NOx emission modelling lies in between one to ten percent. It can be observed in **Fig. 18**, this target was reached at stage 6 (MV-6) with a relative error of 9.4%, and thus, the process was terminated. However, subsequent iterations can be carried if further improvement is required. The identified response surface model at sixth iteration was based on a mapping DoE of 150 MB and 20 MV test points. This is significantly less than normal stationary mapping DoEs, which typically use 120-150 (at each steady state speed and load minimap points) test points [41].

The illustration of NOx emission response surfaces through stage 1 (MV-1), and stage 6 (MV-6) is presented in **Fig. 19** and **Fig. 20** respectively. These figures depict the changes in the response surface, shape and trend, of NOx emission through the iterative process of sequential design of experiments. With the increase in the number of test points, the prediction accuracy of the model improves throughout the design space. The major improvement in between MV-1 and MV-6 response surface can be observed at the extremities of the design space. In **Fig. 19**, the design space of stage 1 is deficient at low load region at both low and high engine speed. With the increment in infill points, it can be observed the corners of the design space has extended to cover the low loads, and the prediction accuracy has also improved. In **Fig. 20**, there is a clear trend that the concentration of NOx in the engine out emission increases as the load increases. The increase in load is a result of vigorous combustion which results in increased in-cylinder pressure and temperatures, leading to increase in the NOx. Also, as the load increases less amount of exhaust gas is recirculated by the EGR system. Recirculating exhaust gas into the cylinder leads to lower combustion temperature and reduced amount of oxygen available in the cylinder, hence less engine-out NOx.

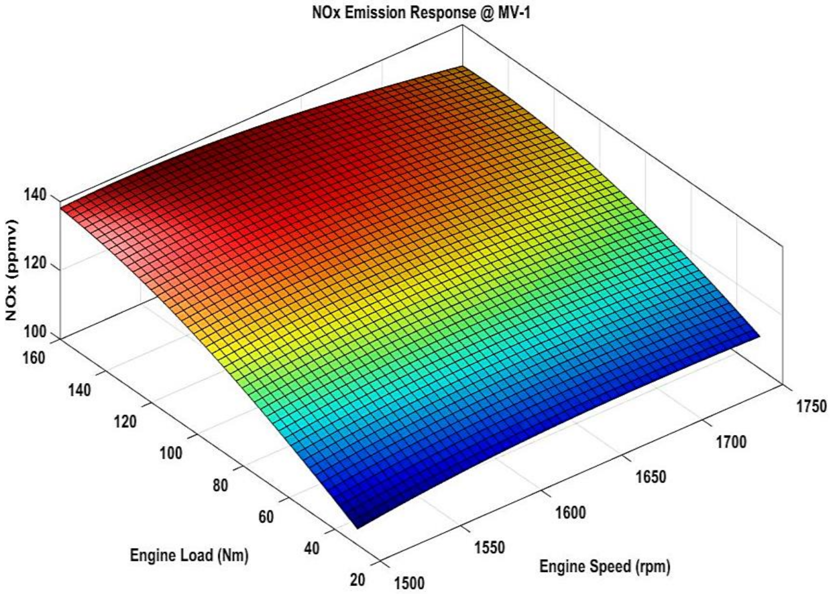


Fig. 19. GPM NOx surrogate response surface model at MV1 stage.

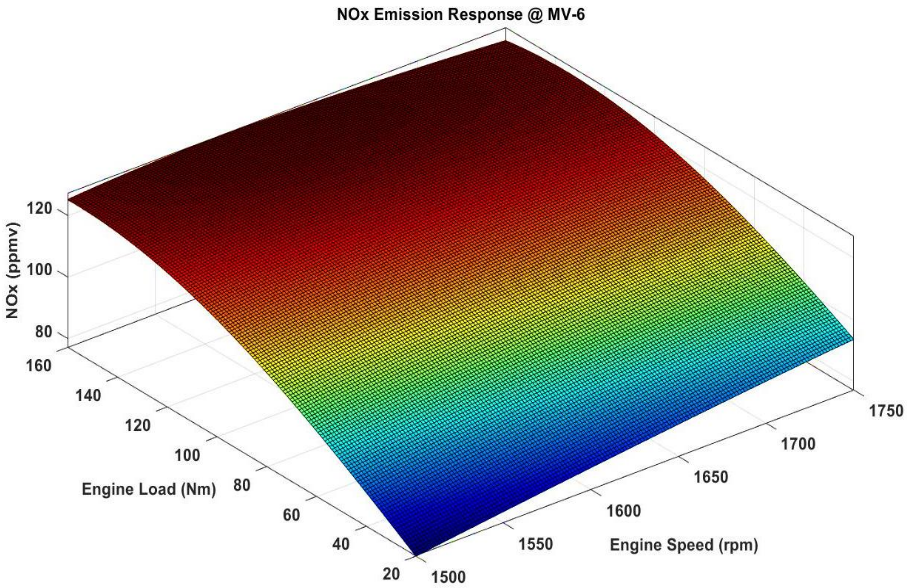


Fig. 20. GPM NOx surrogate model response surface model at MV6 stage.

6 Hybrid Dynamic Modelling Framework Validation

The final stage in this study was to evaluate the performance, in terms of effectiveness and efficiency, of the hybrid dynamic modelling approach. This was carried out by evaluating the performance of hybrid dynamic modelling approach on the transient drive cycle.

The regions of the drive cycle which are within the boundaries of the operation domain of the diesel engine case study were selected and are presented in **Fig. 21**. The selected regions are continuous in time, as extracting points which are not continuous points would lead to distortion of drive cycle and the prediction on such points by NOx model would not be comparable.

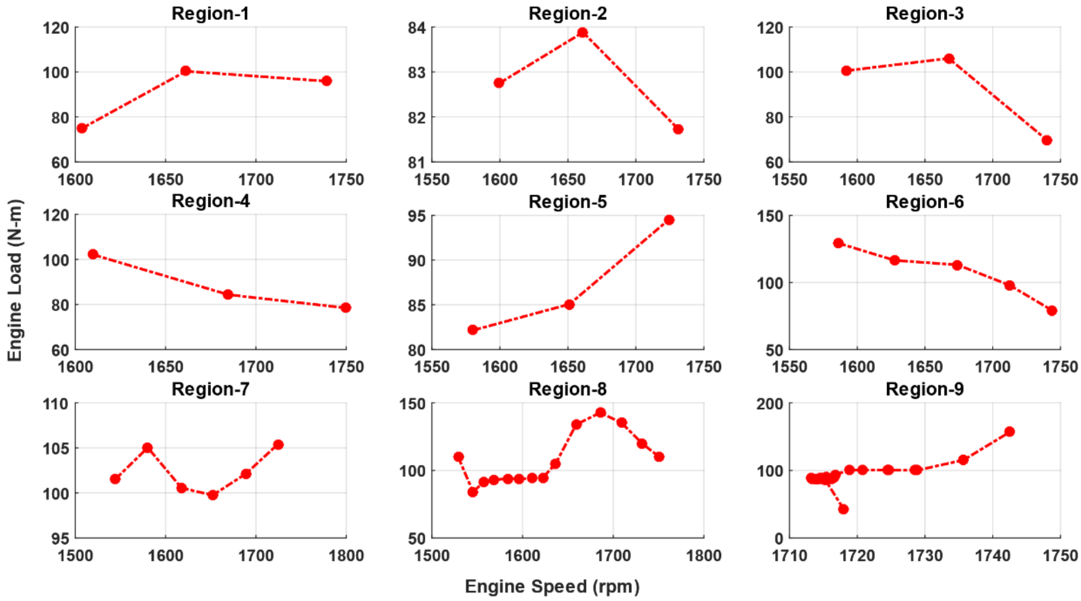


Fig. 21. Selected regions of the continuous point in NEDC drive cycle within the operational boundaries of case study zone.

In this paper, 'Region 9' is selected to present the model performance, as this region had the longest length of the continuous sequence (29 seconds). The performance of the developed modelling framework on region 9 is illustrated in **Fig. 22**. For all the other regions, the corresponding fit statistics have been summarized in **Table 8** and the trend analysis is illustrated in **Fig. 24**.

From **Fig. 22**, it can be observed that hybrid dynamic modelling approach predict the trends, associated with the drive cycle NOx emission, reasonably well.

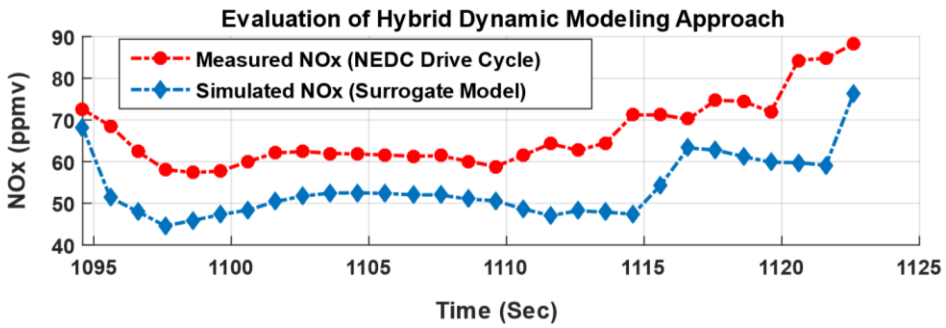


Fig. 22. NOx emission model performance at region 9 of the NEDC drive cycle.

For Hybrid dynamic modelling approach, both the RMSE and relative error are approximately two times the one observed during surrogate modelling. This increase in error can be linked to two main factors:

- As GT suite engine model is a representation of the actual system, it would have an error associated with it. This error is propagated to dynamic models, as the dynamic air path model is developed based on GT-Suite Diesel engine model. During the validation of GT-air path model in [14], it was observed that controller struggles with rapid changes in EGR requirement and some regions of NEDC are predicted with an error. This would explain some of the discrepancy in between measured and modelled response, as it was observed during the sensitivity analysis carried out by authors in [5] that changes in EGR significantly impact the NOx results predicted by SRM model. Additionally, the dynamic air path model which provides inputs for combustion model also has a validation error of 0.014 mf associated with EGR predictions.
- Secondly, there will be difference in between the prediction of emissions from SRM combustion model (MPES platform) and measurements on the test bench, and this error will be introduced into the surrogate NOx model. This would also affect the model capability to measure the absolute values accurately. During the development of the SRM combustion model carried out by the authors in [5] it was observed that the SRM model can accurately capture the trends but underestimates the NOx concentration in the case study domain. The

experimental NOx (measured on test bench) and the simulated NOx (SRM combustion model) were compared during SRM model development in [5] and the observations are illustrated in **Fig. 23**.

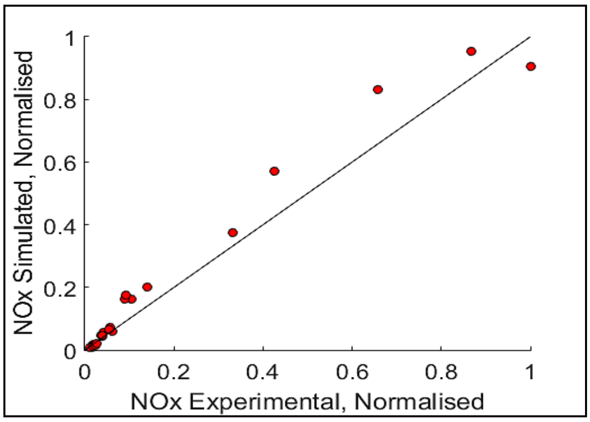


Fig. 23. Simulated NOx (SRM combustion model) versus experimental NOx (measured on test bench) at calibration reference points.

Although the relative error in region 9 is higher than expected but the average relative error across all the nine regions was observed to be 13.7%, refer to **Table 8**. Also, it can be observed from **Fig. 24** that the trends predicted by surrogate NOx model for other selected regions is similar as for region 9.

In literature there are studies [2,21,27], which have been able to estimate NOx emission using dynamic modelling techniques in a range of 5 % -10%. However, in these studies the models were fitted to the test bench data or virtual engine calibration was developed using dynamic modelling techniques based on test bench data. Given that the NOx predictions in this work are based on a virtual engine model, with uncertainty about some important parameters (like the injection profiles, actual EGR etc.), and that the objective of the work is to provide prediction capability for early engine development stage, the accuracy of predictions can be considered adequate.

Table 8. Statistical performance of both surrogate models (hybrid dynamic modelling and steady-state approach) across all the 9 regions.

Region	RMSE	% Relative Error
Region 1	13.09	18.01
Region 2	1.35	2.30
Region 3	13.8	20.35
Region 4	3.07	5.66
Region 5	9.74	14.99
Region 6	5.20	7.05
Region 7	4.09	5.87
Region 8	8.56	11.480
Region 9	13.94	20.93
Weighted Average	**9.33**	**13.67**

Based on the analysis carried out for hybrid dynamic modelling, the proposed approach provides significant improvement both in terms of capturing trends and accuracy. Although the data on which comparison is carried out is small, the hybrid dynamic modelling framework exhibit enormous potential for simulating drive cycles in real time while providing reasonable accuracy.

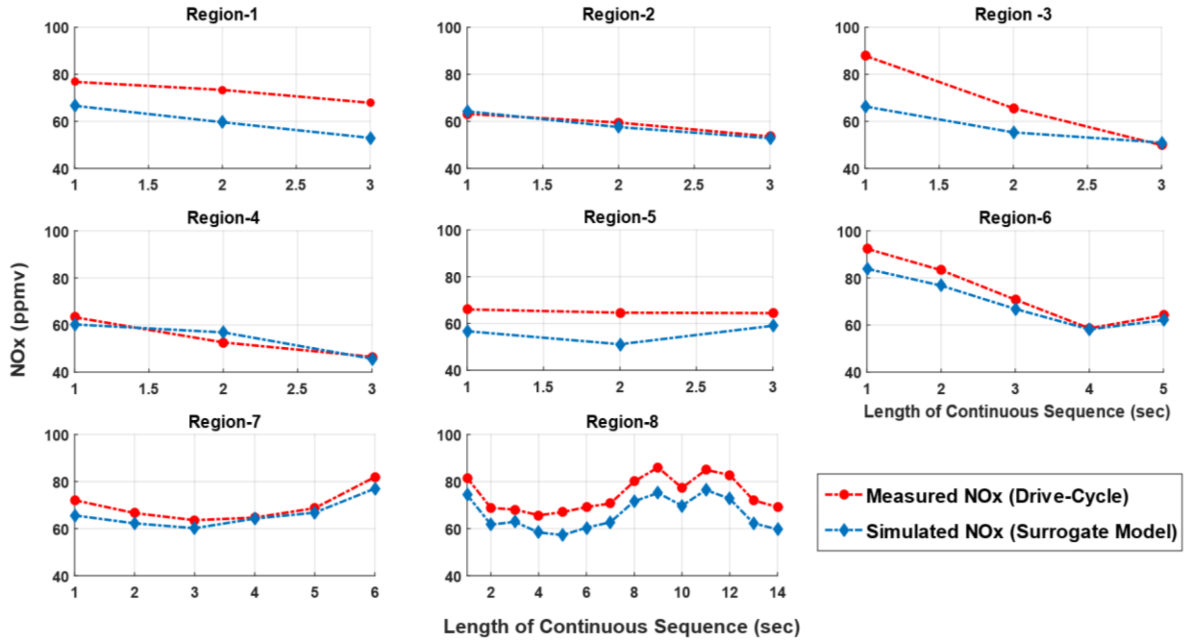


Fig. 24. NOx Surrogate Model response over the selected regions of transient drive cycle.

7 Conclusion

The main aim of this paper was to introduce a novel hybrid dynamic modelling framework to enable the development of a global metamodel of engine emissions. The hybrid methodology, coupling dynamic modelling with a global exploration-based DoE on a multi-physics virtual engine simulation platform, was proved to be an effective approach to develop an engine emissions model that has transient cycle simulation capability during early stages of engine development.

The use of nonlinear dynamic models enabled the development of global metamodel of emission at a comparable cost to steady-state experiments performed to develop the SRM surrogate model by providing fast mean value estimate for the inputs required for SRM combustion process model. It was observed that surrogate dynamic model can provide inputs for SRM model 210 times faster than it would have taken for GT model to run to reach stable steady state operation. Also, with the incorporation of global exploration DoEs based on space-filling OLH DoEs, the number of measurements required to capture the transient behavior of the system was considerably reduced when compared to steady-state point-based approach. The surrogate NOx model was fitted using 150 model building test points and validated on additional 20 test points.

Integration of the dynamic surrogate models for GT-Suite Diesel engine model and statistical models (developed based on data collected using global exploration Doe approach) for SRM combustion process model can enhance the modelling of engine emissions, through delivering high quality models fulfilling the target model accuracy with faster simulation time and reduced number of measurements. As illustrated in the case study (**Fig. 24** and **Table 8**), the NOx surrogate model (developed based on a simulation model) fitted using 150 test points was able to follow the trends observed in the transient drive and was able to do so with associate RMSE of 9.33 ppmv (parts per million by volume) which translates to a competitive 13.7% relative error (ratio of RMSE to mean of measured NOx). The accuracy, of the surrogate NOx model for prediction for drive cycle NOx emissions, whether it is acceptable or not would depend on the development stage. However, given that the modelling error (during the development of surrogate combustion model) was observed to be 9.64%, in **Fig. 18**, the relative error of 13.7% in between simulated and measured drive cycle NOx emission is within reasonable limits. This reflects on the effectiveness of the developed hybrid dynamic modelling framework. While the accuracy achieved for the design space chosen as scope for the validation experiments in the present case study was deemed satisfactory for the purpose of early engine development work, these models might not be of sufficient accuracy to support detailed tuning work on other parts of the system such as after treatment system control. The accuracy of the models can be improved by increasing the number of iterations, as this will increase the infill points within the design space and the boundary, while also employing a hybrid intelligent learning performance metrics to avoid overfitting.

Secondly, by exploring the option of improving the SRM model prediction fidelity through investigation of multi-zone SRM models.

This study demonstrated that the proposed hybrid dynamic modelling framework could provide a trade-off between system modelling accuracy and development time. Although the hybrid dynamic modelling approach provides a feasible solution to some of the challenges in the industry, further work is needed regarding its application. The work presented here by the authors has been a proof of concept for the proposed hybrid dynamic modelling approach, therefore has only been applied and validated on a limited operating range (one zone, i.e. 1500-1750 rpm). This needs to be addressed in the future work by extending the modeling work to capture the entire engine operating domain, such that it can be established that methodology could work with other regions given the relevant data is available. Furthermore, the framework needs to be validated on other dynamic cycles such as WLTP (Worldwide Harmonised Light Vehicle Test Procedure), RDE (Real Driving Emissions) test or FTP (Federal Test Procedures). This will strengthen the argument that the approach developed here offers the possibility to be incorporated into engine calibration, since it allows fast data capture and reduced measurement effort, thus, the less experimental effort required (compared to traditional point-based calibration).

We envisage that the proposed hybrid modelling methodology will be of broader interest for application in other areas given the increase use of multi-physics simulations, as well as for dynamic physical or hardware-in-the-loop (HiL) based testing and analysis, to support faster and cheaper modelling and calibration experiments.

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